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Westminster, Colorado, USA

Evaluating perspectives from past missions to shape future investigations using the Mars 2020 Planetary Instrument for X-ray Lithochemistry

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Mars 2020 Project

XRF in Planetary missions

NASA Contact science missions Mars employing XRF

- **Viking 2** (1975) — ^{209}Cd, ^{55}Fe
- **Pathfinder** (1996) – Sojourner — APXS
- **MER** (2003) – Mars Exploration Rover – Spirit and Opportunity rover — APXS
- **MSL** (2012) – Mars Science Laboratory – Curiosity rover — APXS
- **Mars** 2020 – Planetary Instrument for X-ray Lithochemistry (PIXL) — Rh X-ray tube

NASA Contact science missions employing XRF

- **Venera 13/14, VEGA 2** (1983/84) – Venus — ^{238}Pu, ^{55}Fe
- **PHILAE Lander** (2014) – comet 67P/Churyumov-Gerasimenko — APXS
- **VIXL** – Venus Instrument for X-ray LIthochemistry Rh X-ray tube – Venus — APXS?
- **Moondiver** (20??) – The Moon — APXS?

Viking Lander program

- Landers - Viking 1 (Chryse Planetia) and Viking 2 (Utopia Planitia)
- Launched 1975
- First Mars landers
- Spectrometer: ^{55}Fe (5.9 keV) and ^{109}Cd (22 keV) radioisotopes, proportional counter
- Rock chemistry, atmosphere, signs of life, images

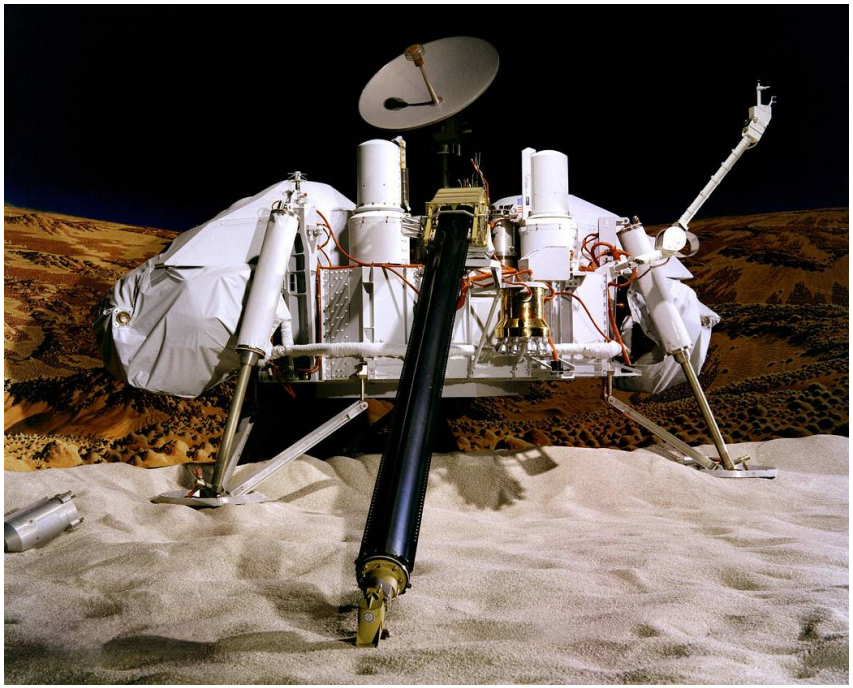


Figure: Viking lander model. Source: https://www.nasa.gov/sites/default/files/images/585497main_PIA09703_full.jpg

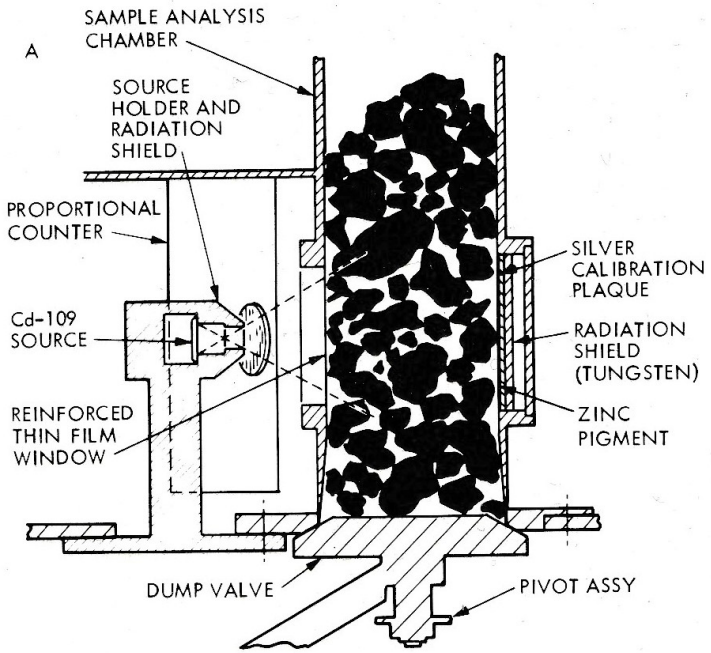


Figure: Schematic of Viking lander sample analysis chamber. Source: https://www.nasa.gov/sites/default/files/images/585497main_PIA09703_full.jpg

Viking 2 Lander - findings

- Spectrometer resolution – 1000 eV @ 5.9 keV FWHM
- Weathered basaltic lava
- High **Fe** and Al, Si, K, Ca, Ti
- Very high **S** and **Cl** – ocean precipitates
- Rb, Sr, Y and Zr traces
- Soils same on both sides of planet (wind storm distribution)

Deliverable

- First in-depth look at surface chemistry
- Co-validation of later data

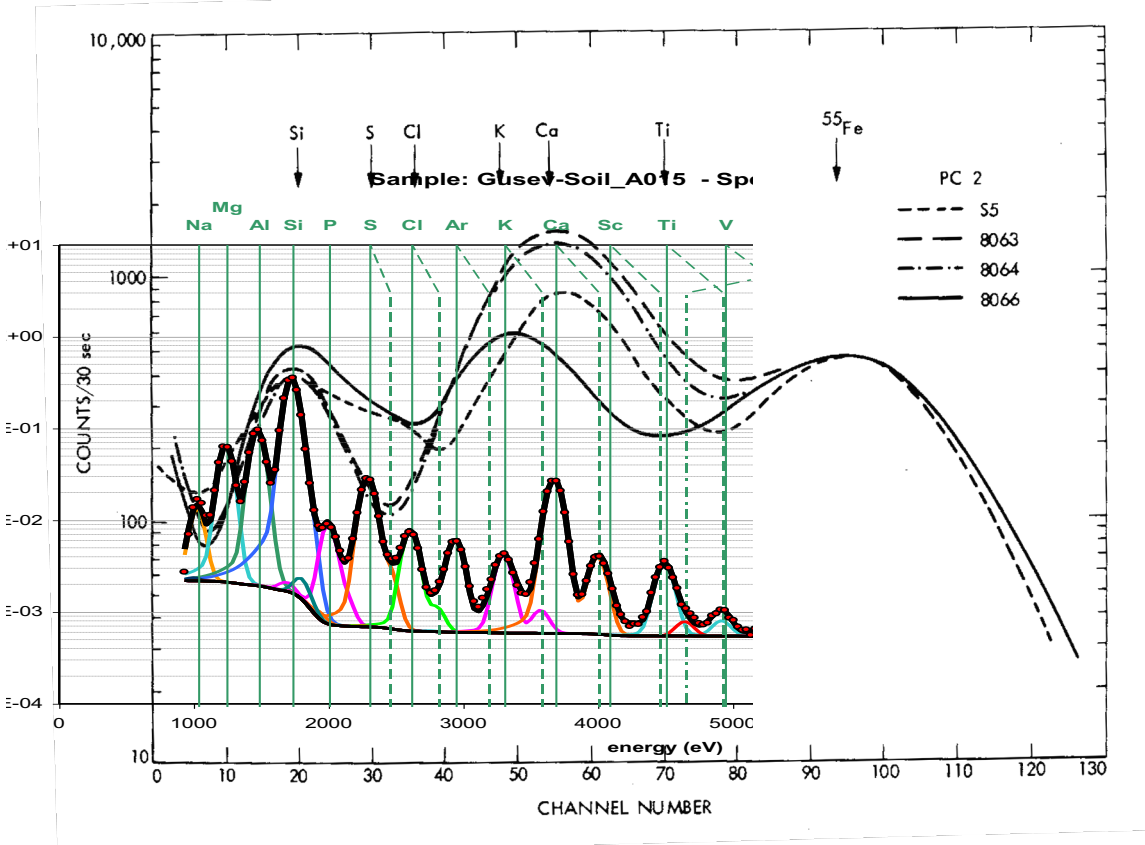


Figure: Overlay of Viking measured soil spectrum with example APXS spectrum.

Mars Pathfinder Mission

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

- Rover "Sojourner" – launched 1996
- Landing Site: Ares Vallis
- First rover and airbag landing
- APXS – Alpha-proton X-ray Spectrometer
  - ~250 eV @ 6.4 keV

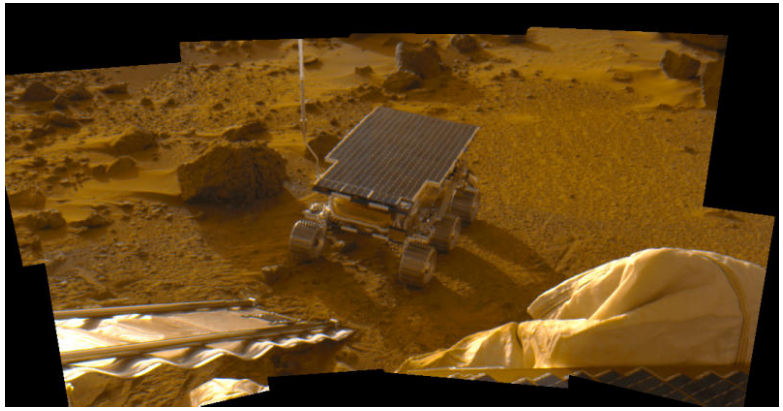


Figure: View of Sojourner rover source: https://www.nasa.gov/specials/pathfinder20/

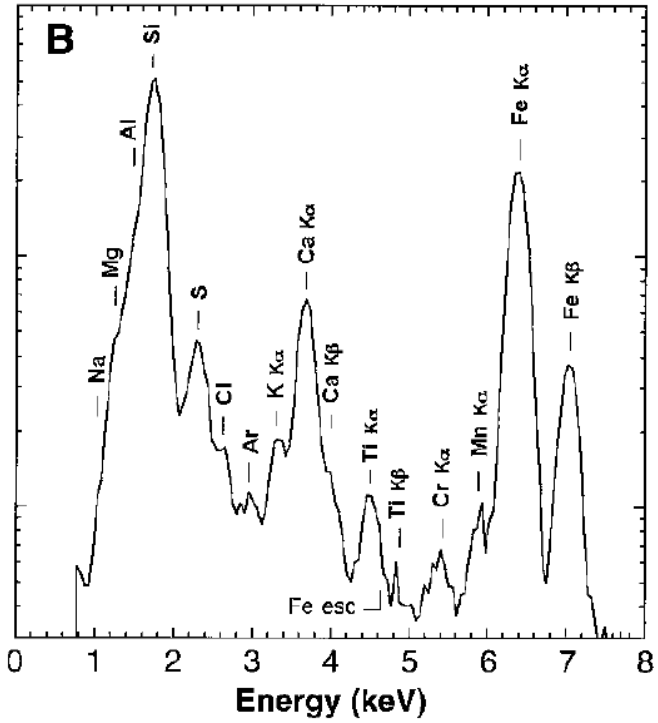
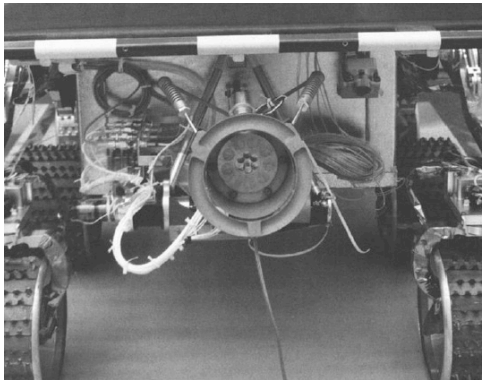


Figure: Pathfinder APXS spectrum of A-15 dark soil at Mermaid Dune site. Source: Rieder et al. 1997b Science **278** 1771-1774.

Discoveries

- Evidence of lakes and running water – Pebbles
- Mars Radius
- Atmospheric data
- Bulk Mars soil composition – similar to Viking. [S] and [Cl] differ.

Figure: Pathfinder APXS mounted on rover. Source: Rieder et al. 1997a J. Geophys. Res. E **102** 4027-4044.



Mars Exploration Rover (MER)

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

- Spirit and Opportunity Rovers – launched 2003
- Landing Sites: Columbia Memorial Station – Spirit, Meridiani Planum – Opportunity
- Opportunity – Active (2004 – present)
- Past water activity, rock chemistry, habitable regions
- APXS resolution – 160 eV @ 5.9 keV
- E cutoff – 16 keV

Figure: View from Cape Tribulation on rim of Endeavour Crater, Jan. 22, 2015. Source: https://www.jpl.nasa.gov/spaceimages/details.php?id=pia19109

Figure: MER rover in high-bay at JPL. Source: https://mars.nasa.gov/mer/gallery/spacecraft/images/liverover.jpg

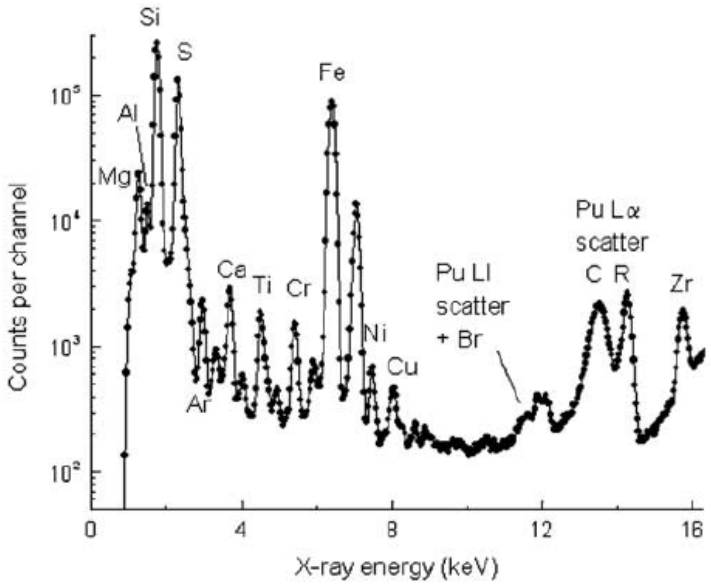


Figure: MER APXS spectrum of high-sulfate soil. Source: Campbell JL et al. (2008) J. Geophys. Res. **113** E06S11.

Discoveries & Comments

- Sulfates – hydrated [H2O] – Compton-Rayleigh
- Gusev
  - Outside rock coatings and cracks –water flow
  - Nickel – meteroites
- Columbia Hills
  - P, S, Cl, Br enrichment – aqueous alteration
- Clays, pure silica, carbonates – water exposure.
- "blueberries" – contains hematite

Mars Science Laboratory (MSL)

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

Figure: Artistic rendering of rover descent via skycrane. Source: https://www.nasa.gov/mission_pages/msl/multimedia/gallery/pia14839.html

Curiosity Rover – Launched 2011 – Gale Crater

Mission: Habitability and humans to Mars

- Organic compounds
- Biosignatures
- Surface radiation
- Geological history

Figure: MSL Rover self image taken on Mount Sharp. Source: https://photojournal.jpl.nasa.gov/catalog/PIA19808.

Findings: Mars could have supported life

- Volcanic rocks - weathering
- Organic element building blocks
- Methane found
- Strong further evidence of water
- Cold, wet conditions prevailed
- Martian dust – high S & Cl

Mars Science Laboratory (MSL) – cont'd

- APXS – scientific methods development – MSL scientists
  - Relief effects
  - Oversampling - chemical lithology
  - Mineral phase effects (Na, Mg, Al, Si)
  - X-ray diffraction
  - C/R –ratios – "invisible" elements
  - Characterizing detector non-linearity – fits

- APXS properties:
  - Resolution (140 – 180 eV)
  - Full Pu L X-ray line energy range – improved C/R ratios

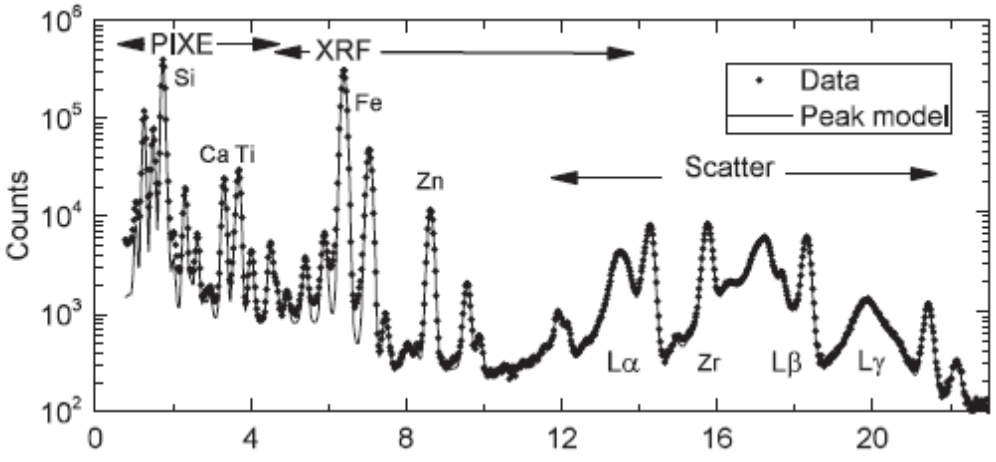


Figure: MSL APXS spectrum of a Martian soil. Source: Campbell JL et al. (2016) Nucl. Instrum. Meth. B 383 (2016) 143 – 151.

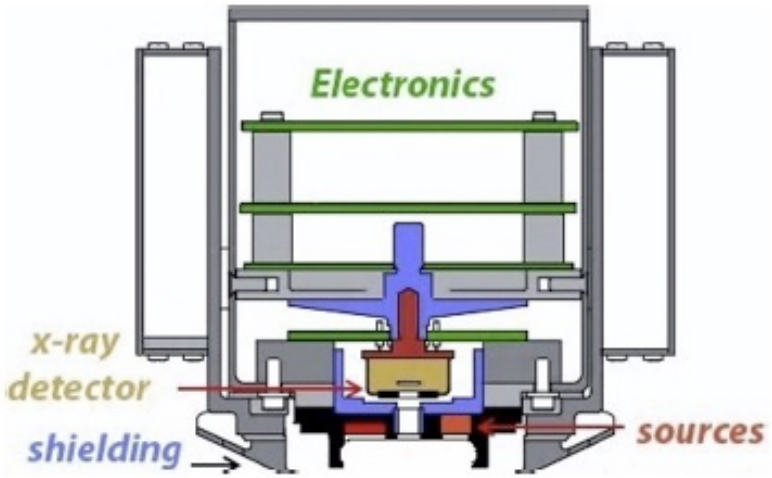


Figure: schematic of MSL APXS. Source: Campbell JL et al. (2013) Nucl. Instrum. Meth. B. **302**, 24 – 31..

Perspectives

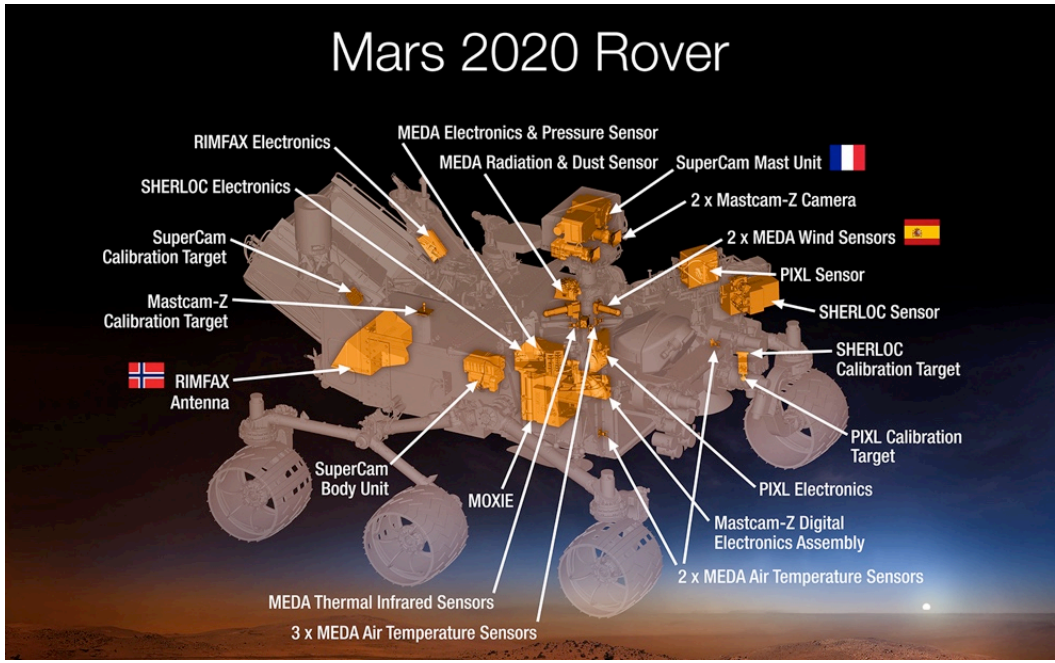
- APXS method – trustworthy, heritage reliability
- APXS techniques – becoming advanced

- Geology and planetary chemistry – ongoing
- Habitability and biosignatures – more searching to be had
- Sub-mm scale probing – uncover individual grain chemistry

Mars 2020 Mission Overview

Mars 2020 Science Objectives

- **Habitability** – past relevant environments
- **Biosignatures** – preservation potential
- **Sample caching** – potential future return
- **Prepare for humans** – *in situ* resources



Mission life: 1.5 Mars years
(1005 earth days)

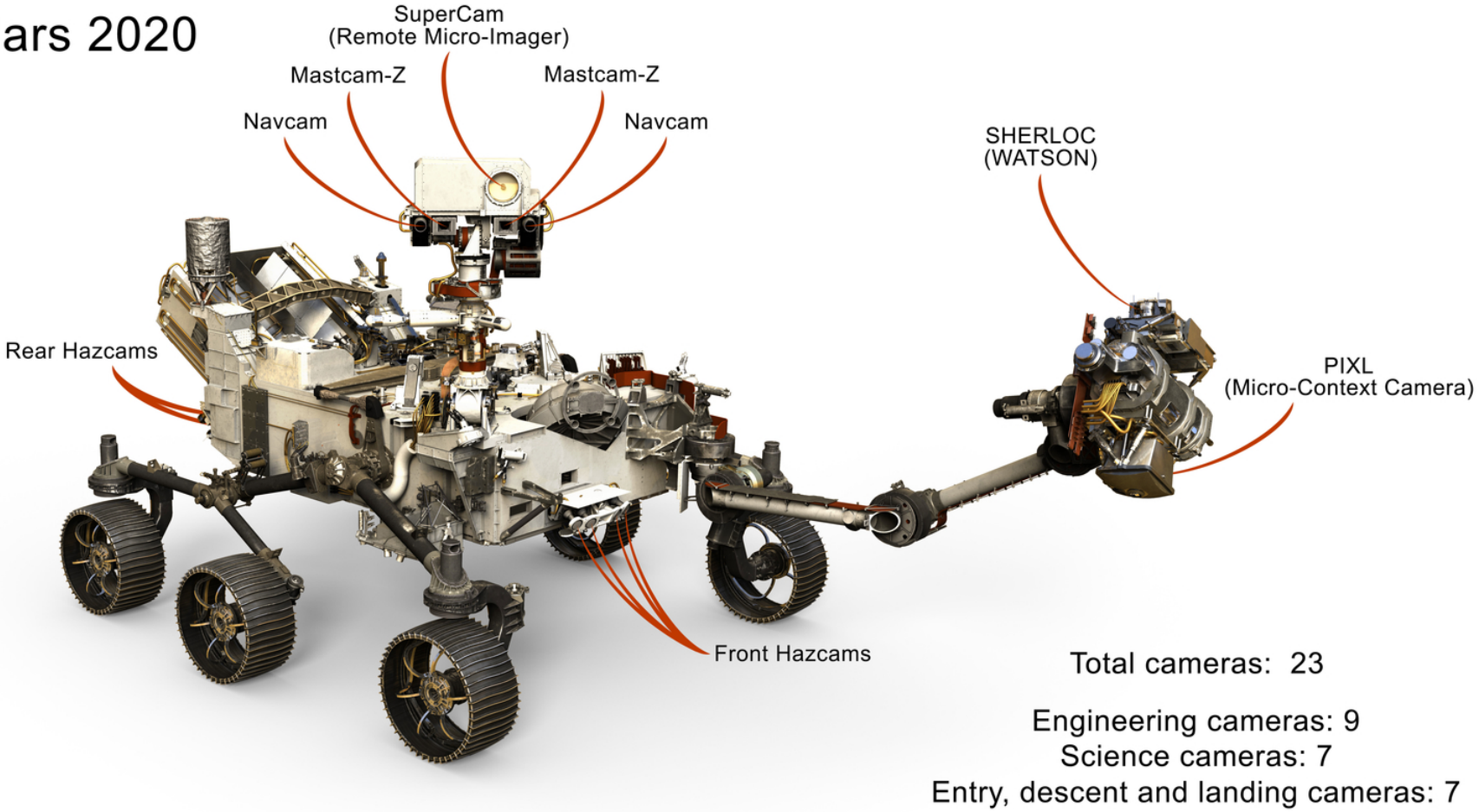
Launch: July, 2020
Land: February, 2021

Instrument Complement:

- Mastcam-Z and Supercam for panoramic/stereo imaging and chemical analysis (LIBS)
- MEDA for weather
- RIMFAX ground penetrating radar
- MOXIE technology experiment to produce Oxygen from CO_2
- SHERLOC and WATSON for UV Raman and high resolution imaging
- **PIXL micro-XRF spectrometer and Micro Context Camera (MCC) imager**

Intro to PIXL

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

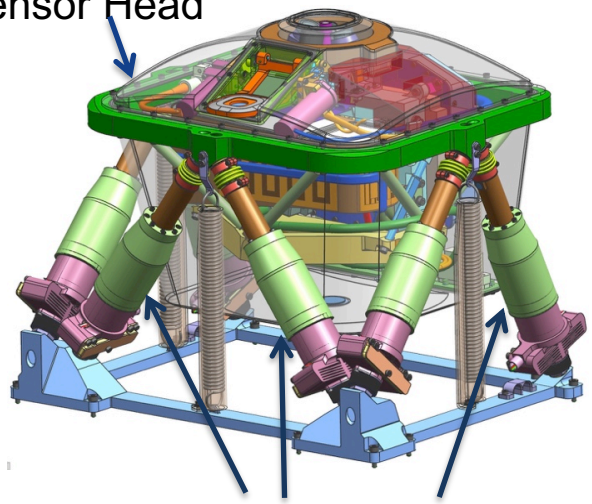


Total cameras: 23

Engineering cameras: 9
Science cameras: 7
Entry, descent and landing cameras: 7

Planetary Instrument for X-ray Lithochemistry (PIXL) – Overview

Sensor Head



Active Hexapod System
(6 Active Struts)

Figure (left): PIXL hexapod sensor head showing struts for (x,y,z) adjustments – source: L. Wade (JPL)

Key components:

- Micro-focus XRF
  - maps, lines, grids
- Optical fiducial subsystem (OFS)
  - exact (x,y,z) rock position
  - image co-registration
  - thermal drifting

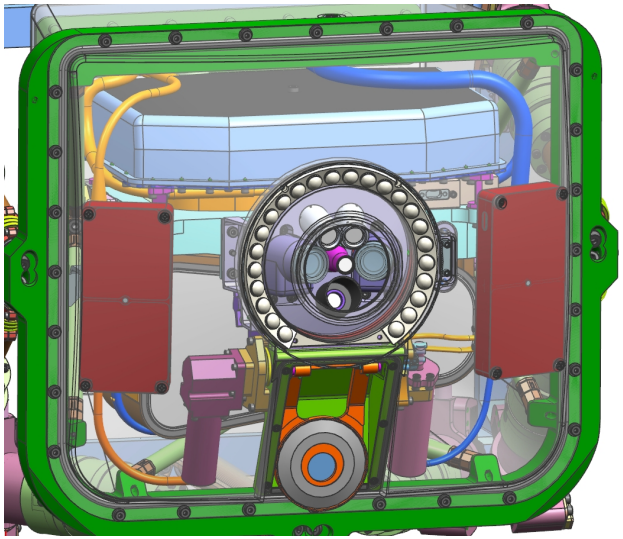


Figure (center): PIXL sensor head front face. Two top cylinders – coarse and fine laser point grids, bottom center – micro-context camera, side circles – two Ketek SDDs, middle - x-ray optic.
– source: L. Wade (JPL)

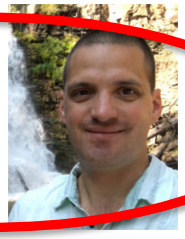
Parameter	Performance Characteristics
Excitation voltage	28 kV
Energy resolution	125 eV @ 5.9 keV
Beam diameter (FWHM)	0.12 mm @ 8.0 keV
Field of View	25 x 30 mm
Step size, any direction	0.06 mm

Table: PIXL operation characteristics – source: L. Wade (JPL)

Core Science Team & Locations

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

Selen Turkay
QUT



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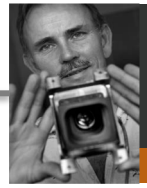
JPL

Abigail Allwood
Principal Investigator
JPL

Joel Hurowitz
Deputy Principal Investigator
STONYBROOK

Yang Liu
Investigation Scientist
JPI



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Tim Elam
Co-Investigator
APL

David Flannery
Collaborator
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Robert Hodyss
Co-Investigator
JPL

Ben Clark
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SSI

Michael Tice
Co-Investigator
U Texas Austin

MCC Team
collaborators
DTU

John Grotzinger
Co-Investigator
CALTECH

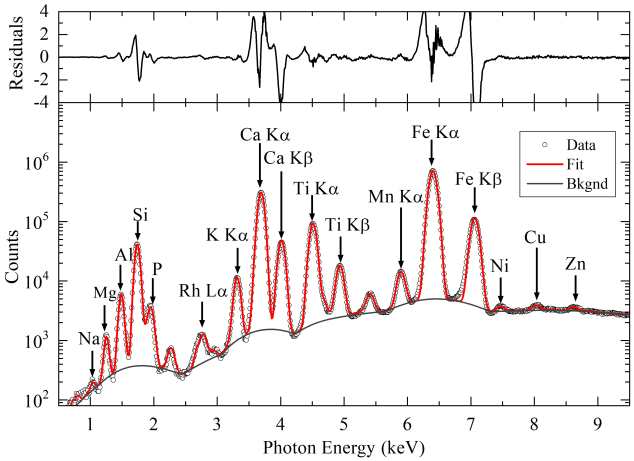
Scott McLennan
Co-Investigator
STONYBROOK

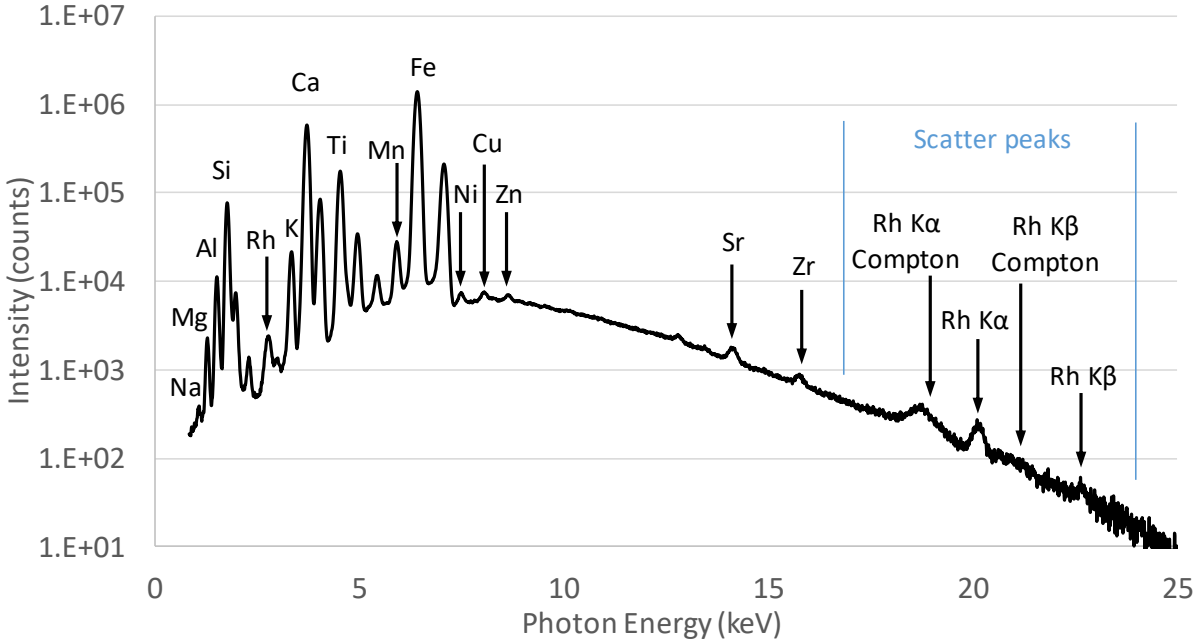
Allan Treiman
Co-Investigator
LPI

PIXL Spectra

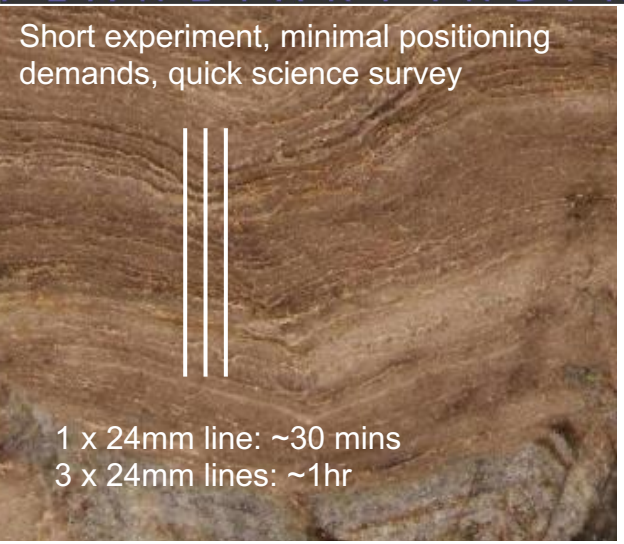
PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

BHVO2 spectra – JPL breadboard prototype

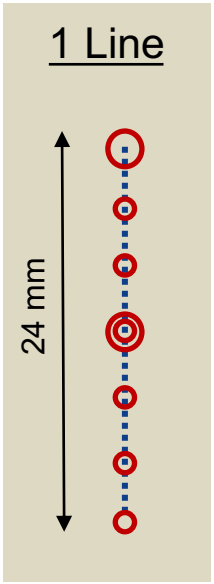


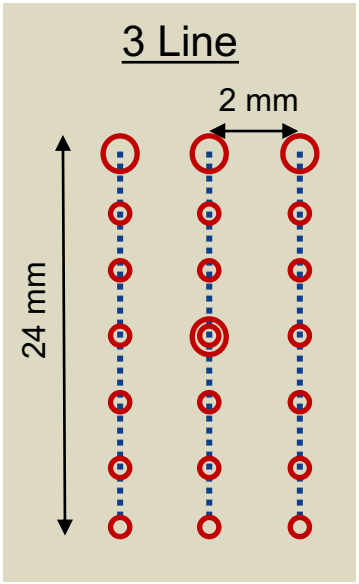


Measurement types: Line Scans



Target: Abraded / Natural
Suits: 1 D heterogeneity / fast survey
Z: Best achievable on natural surface, 25mm on abraded/flat
TOD: Day (typical)
Goal: Summed integration time on each component sufficient to determine the major/minor elements present and their relative variations.



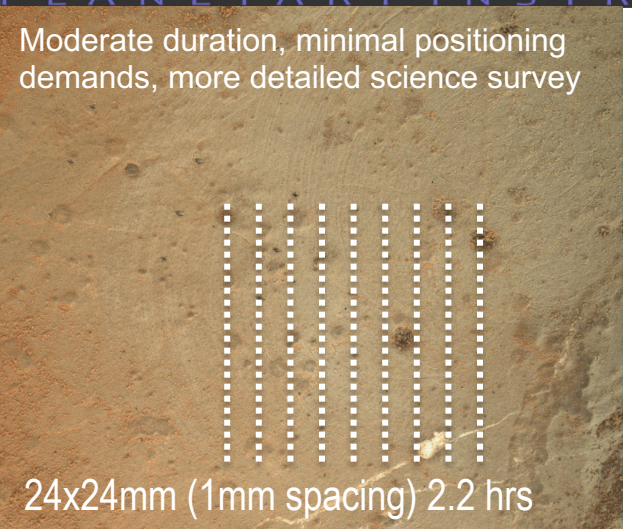


Ops Templates

Step size: 0.12 mm (=beam diameter) along lines
Line length: 24 mm
No. of lines: 1-3
OFS Imaging: Intervals <4 mm, as shown, ensuring continuous coverage of dense SLI pattern for distance determination and X-ray spot location

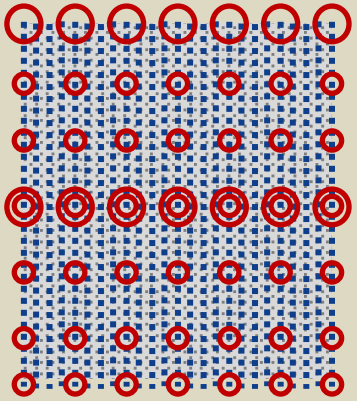
○ Full-sized Image ○ Reduced Image ···· Spectral Line

Measurement Types: Grid



Target: Abraded / Natural
Suits: 2D heterogeneity moderately complex texture scale mm+
Z: Best achievable on natural surface, 25mm on abraded/flat
TOD: Day (typical)
Goal: Summed integration on each component sufficient to determine major/minor elements and relative variations. Quantitative analysis and trace element detection possible on dominant phases

24 x 24 grid

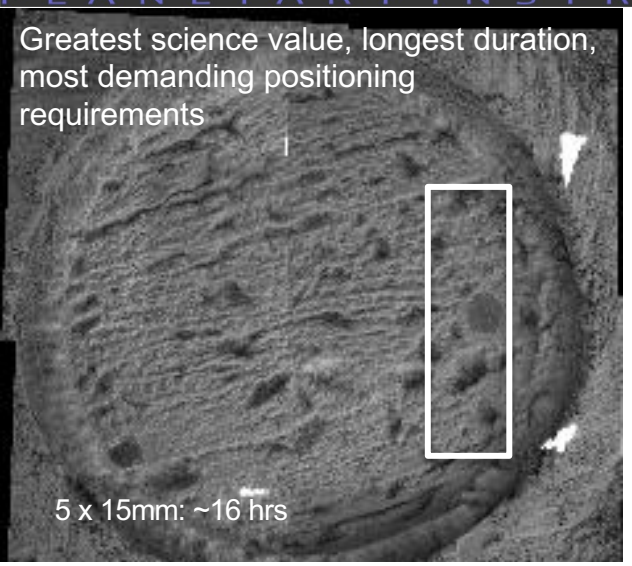


Ops Templates

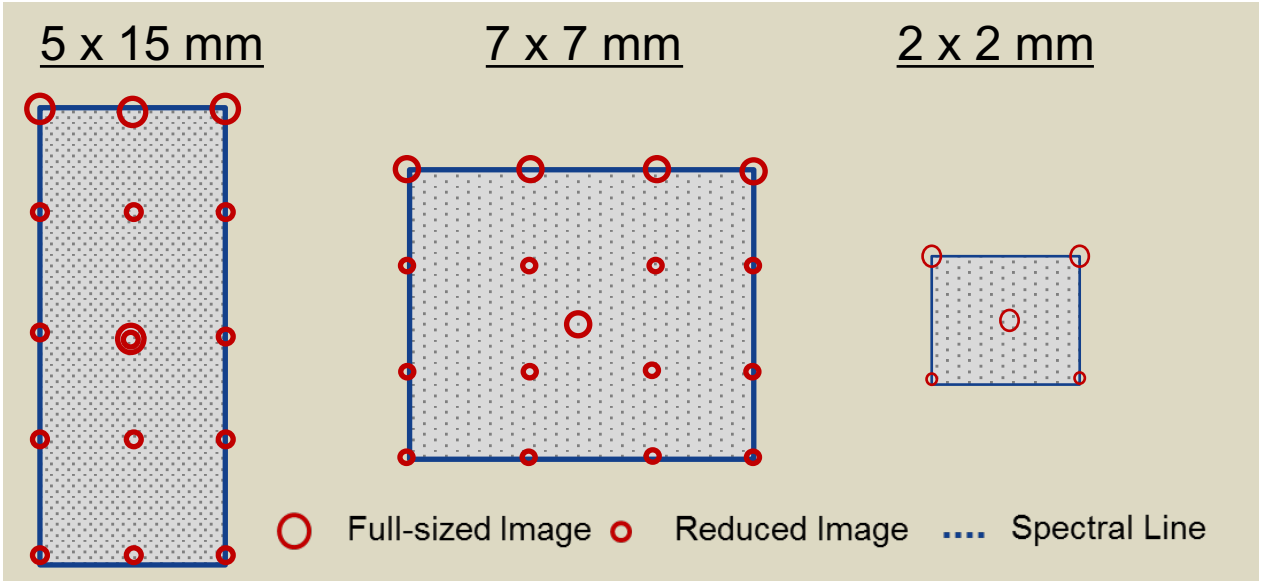
Step size	1 mm (~10 x beam diameter) along lines
Grid size:	24 x 24 mm
OFS Imaging:	Intervals <4 mm, as shown

Full-sized Image Reduced Image Spectral Line

Measurement Types: Map



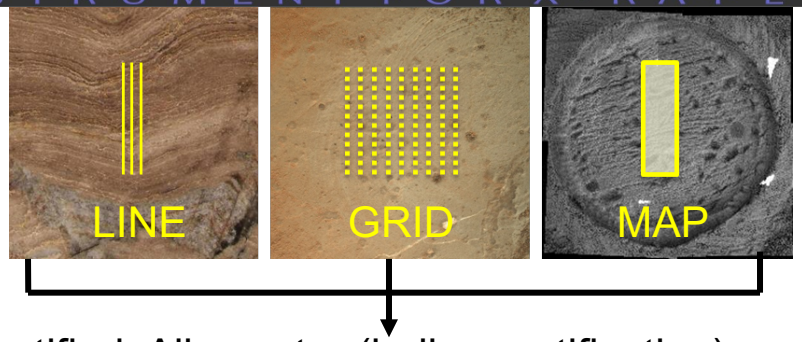
Target: Abraded
Suits: 2D heterogeneity Highly complex, very fine texture, SHERLOC overlap
Z: 25mm
TOD: Overnight
Goal: Summed integration time on each component sufficient for quantitative analysis and trace element detection.



Ops Templates:

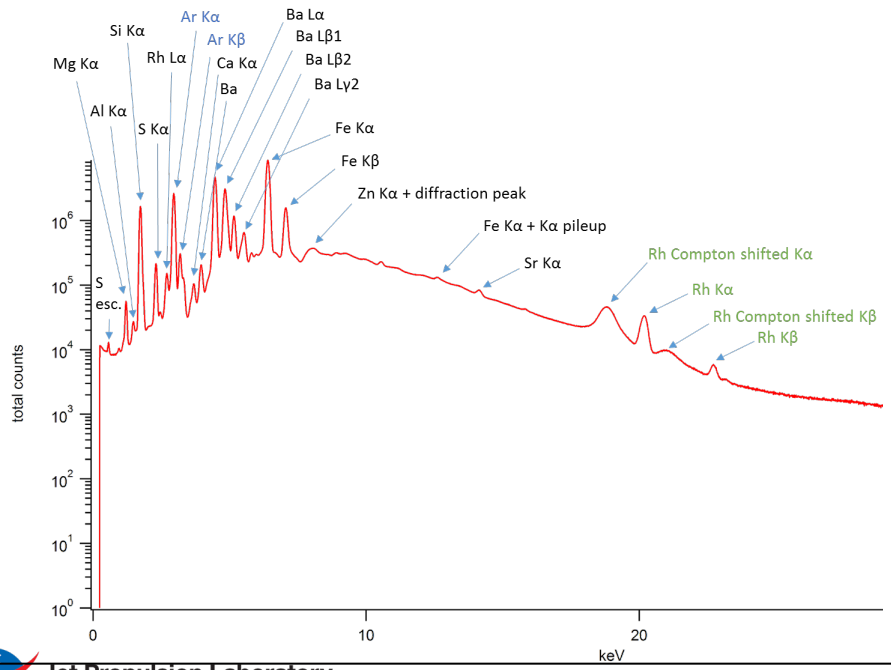
Step size:
0.12mm (beam diameter)
Dimensions:
2 x 2mm,
5 x 15mm
7 x 7 mm

Tactical Data Products: Summed, quantified spectra



Spectra are summed, quantified: All spectra (bulk quantification) and selected rock components. Rock components selected by visible features, or **process shown on next slide**

1. Summed spectrum plot with peak labels



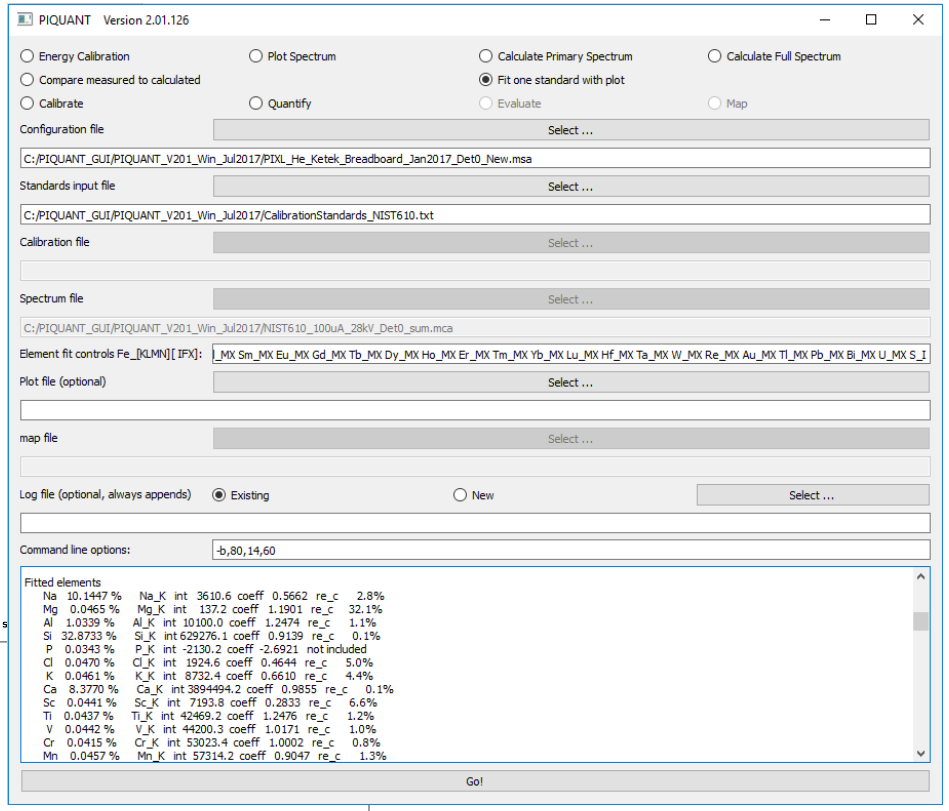
2. Table of calculated abundances

Oxide	Wt % - Comp 1	Wt % - Comp 2	Wt % - Comp 3
Na_2O	7.11	2.08	1.5
MgO	3.61	0.82	5.65
Al_2O_3	16.09	5.66	5.29
SiO_2	50.7	73.65	30.93
P_2O_5	0.49	1.25	0.88
SO_3	2.48	4.8	12.18
Cl	0.87	0.29	1.66
K_2O	2.23	0.96	0.09
CaO	6.07	3.05	25.26
TiO_2	0.49	1.57	0.52
MnO	0.14	0.06	0.87
FeO	9.47	5.49	14.61

PIQUANT processing of PIXL data

Investigation tool (PIQUANT)

- FP
- Optic transmission
- Calculates spectra
- Quantifies (Z)
- **Work in progress**



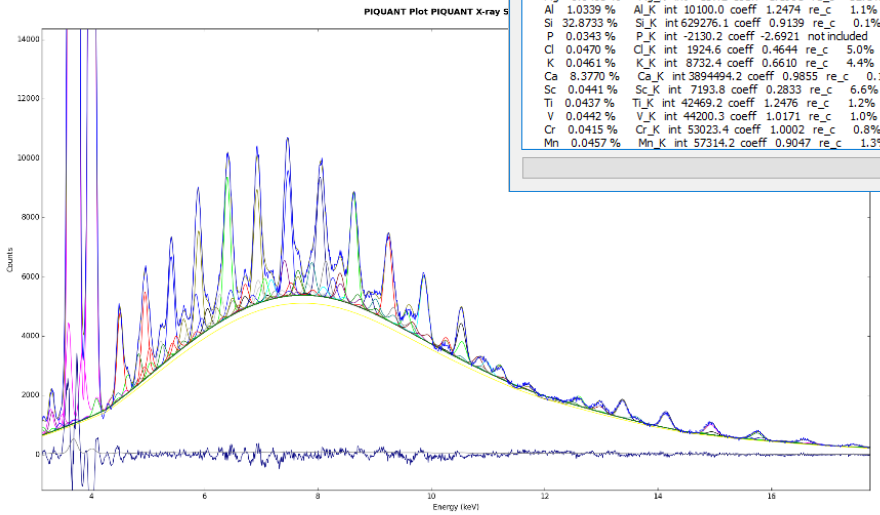
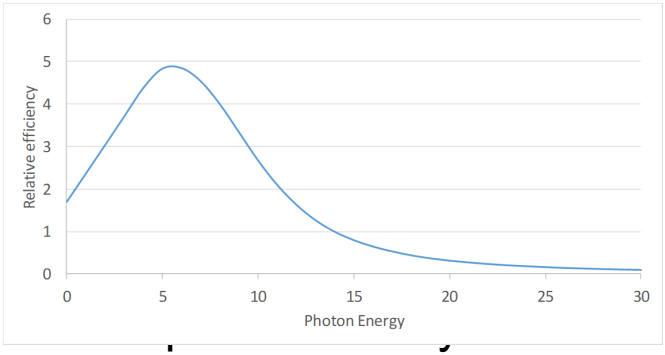


Figure: PIQUANT fitted spectrum of NIST 610 with 60+ trace elements.

- Elam, WT et al. (2002) Rad. Phys. Chem. **63**, 121-128.
- Ebel, H. (1999) X-ray Spectrom. **28**, 255-266.

PIXL optic – Transmission profile derivation

Optic efficiency profile:



- Accuracy → FP approach
- Derive
  - → XRF on H2O
  - → PIQUANT calculated (no tube)

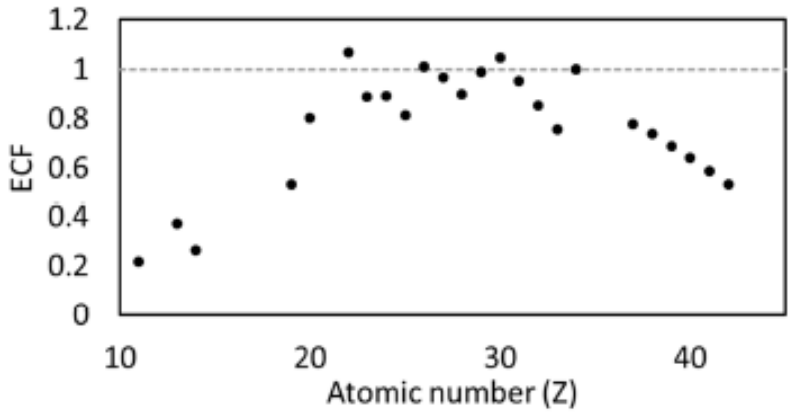


Figure (top): PIQUANT ECF's from fitted spectrum of NIST 610 with 60+ trace elements. Note divergence from unity (1).

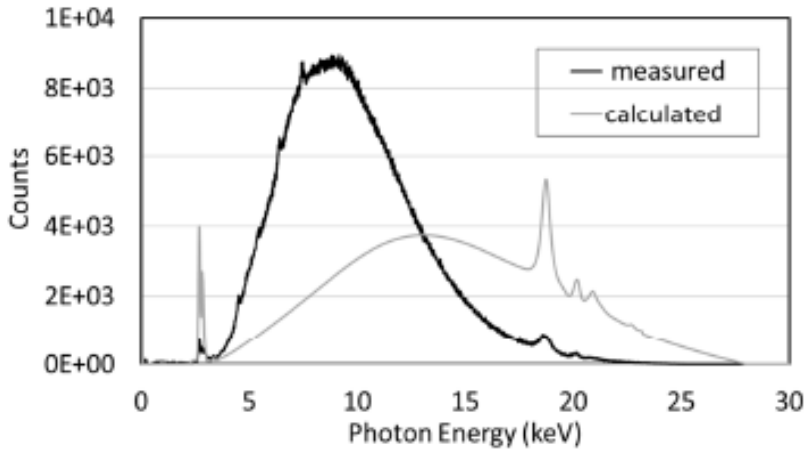


Figure (bottom): Measured and PIQUANT-calculated water spectra.

Optic profile results

- New vs former profile differences
- Mostly corrected ECF trend
  - High Z ECF divergence cause due to fitting issue

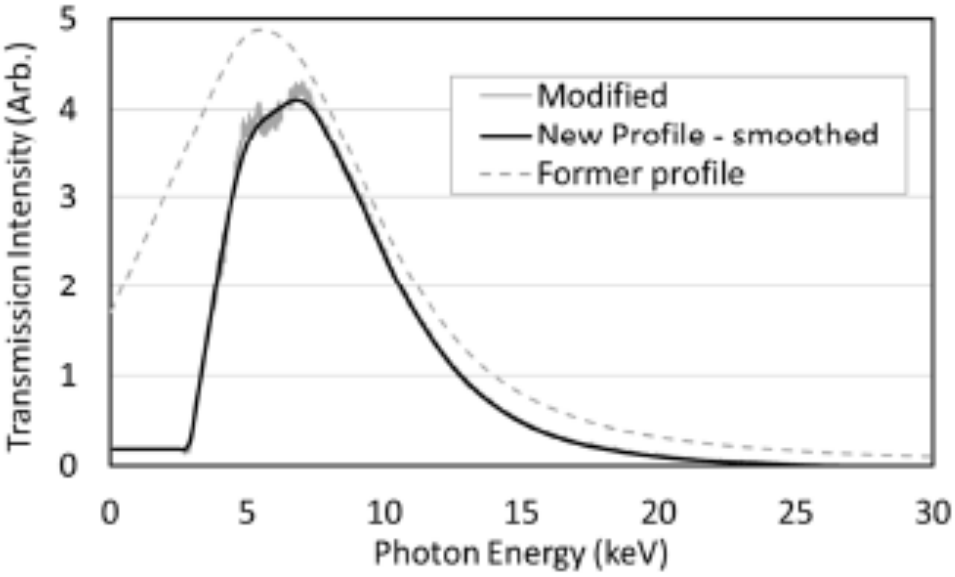


Figure (right): New (smoothed) optic efficiency profile compared against former.
Source: **Heirwegh et al. (2018) Powder Diffraction Journal, 33, 162-165**.

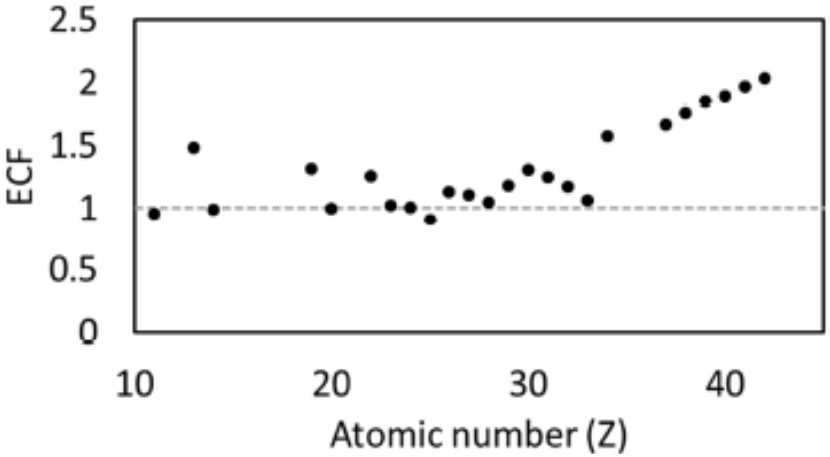


Figure (left): Improved NIST 610 PIQUANt ECF agreement with unity. High Z divergence due to issues with background fit to spectrum.

PIXL Quantification Capabilities

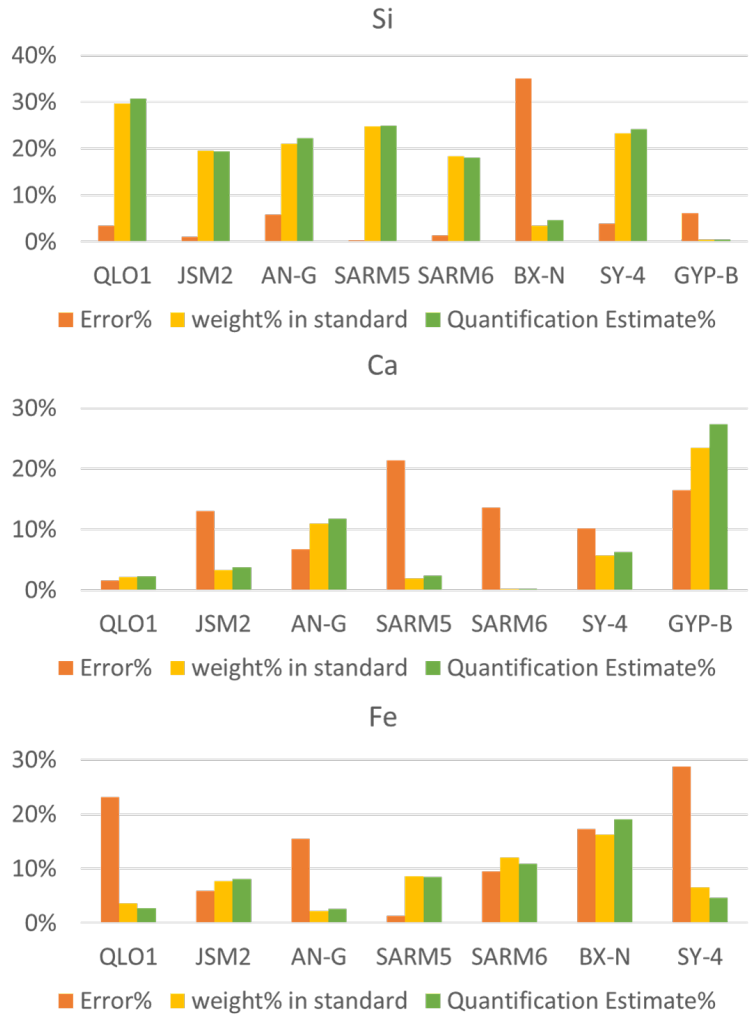
PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

Quantification results:

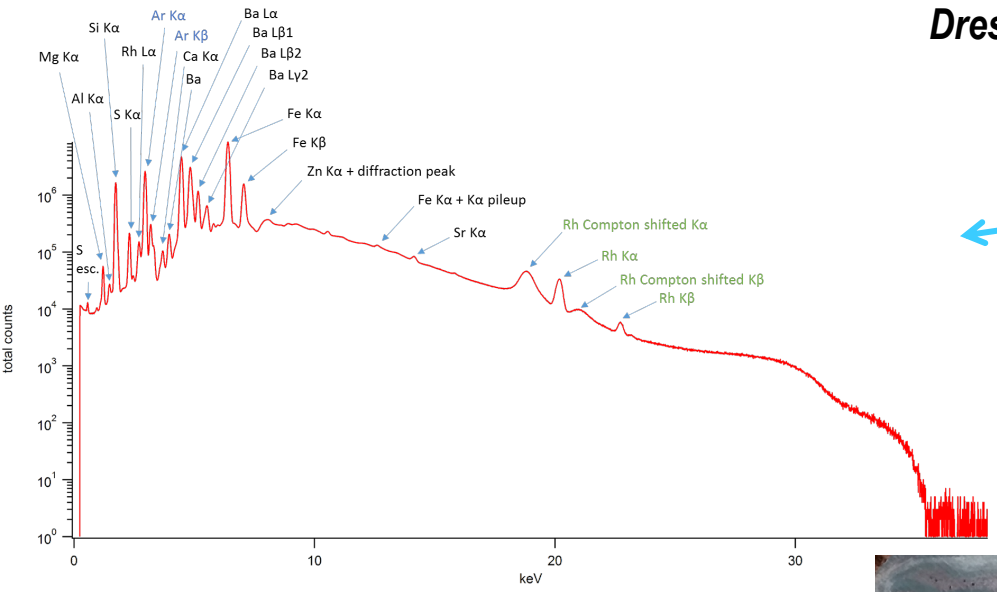
- Informed PIQUANT tasks
- 8 powder standards: QLO1, JSM2, AN-G, SARM5, SARM6, BX-N, SY-4, GYP-B
- Avg error ~10% or better
- Next round – 16 powders

Element	Na	Mg	Al	Si	S	K	Ca	Ti	Mn	Fe
weighted error (%)	9	2	4	2	9	17	4	10	16	7

Table: conc. Weighted error of eight powder certificate values vs PIQUANT concentration estimates.



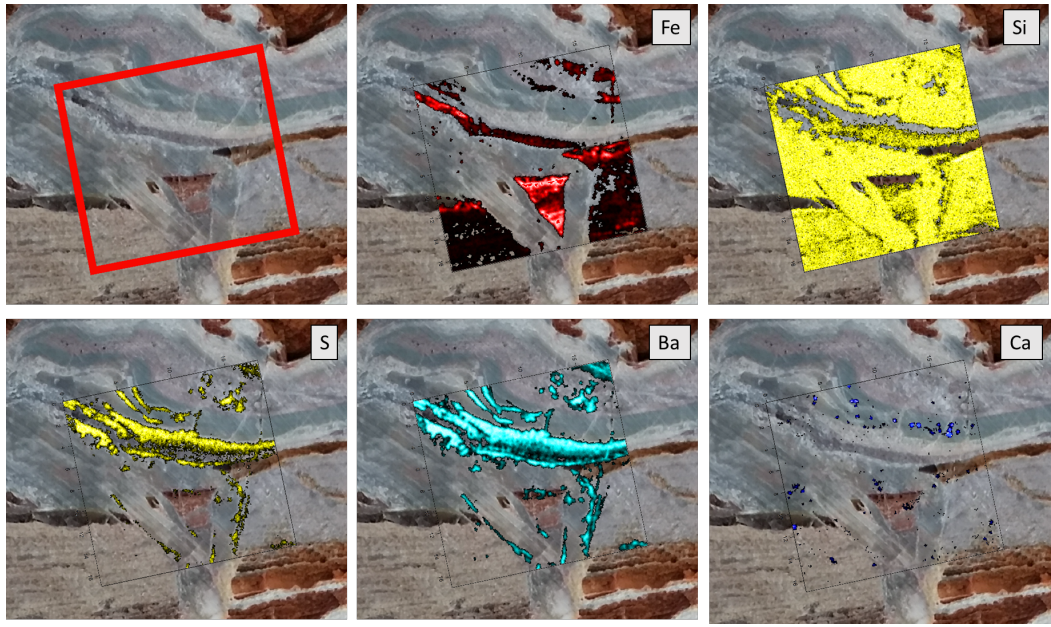
Selecting Rock sub-components



Dresser Formation, Western Australia *~3.5 Ga Microbialites, cross cutting hydrothermal veins, exhalative hydrothermal deposits and multiple modes of alteration*

Bulk Summed Spectrum

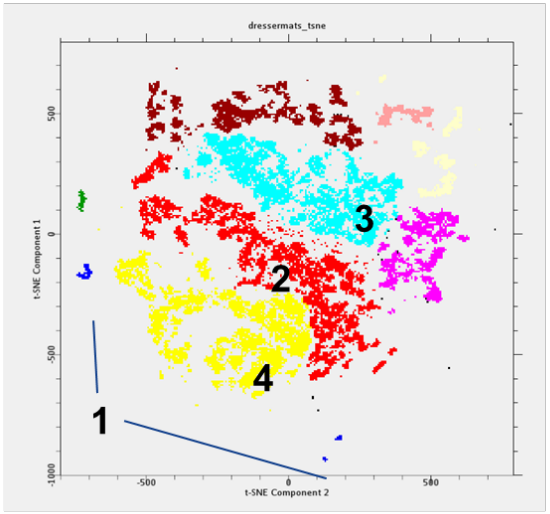
Element Maps (net intensity) for Fe, Si, S, Ba, Ca peaks



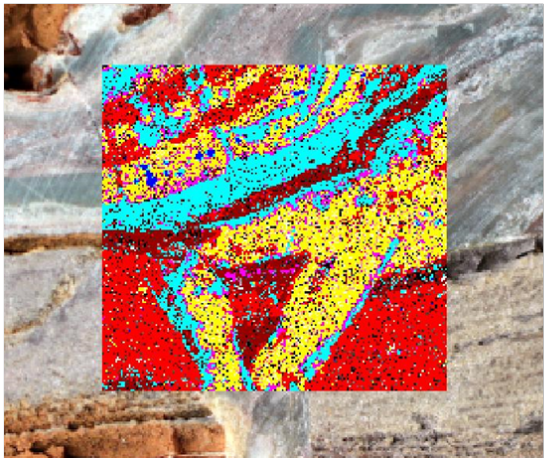
The element maps reveal variations in composition among rock subcomponents. To constrain the elemental composition, lithology and mineralogy of the subcomponents, we must group and analyze spectra from that subcomponent.

Selecting Rock sub-components

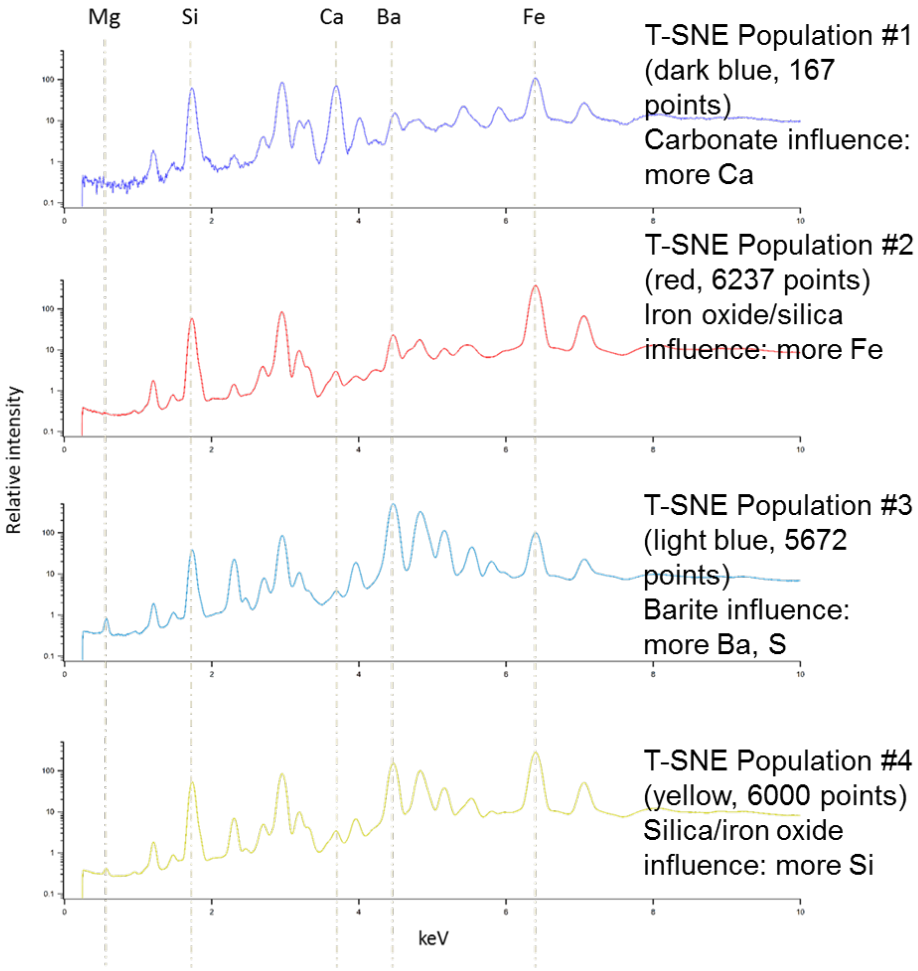
T-SNE (t-distributed stochastic neighbor embedding) scatterplot populations…



…back-projected on a context image



… and sums of the manually selected spectral populations



PIXL: texture-specific chemistry

PLANETARY INSTRUMENT FOR X-RAY LITHOCHEMISTRY

accurate correlation of chemistry with visible textures

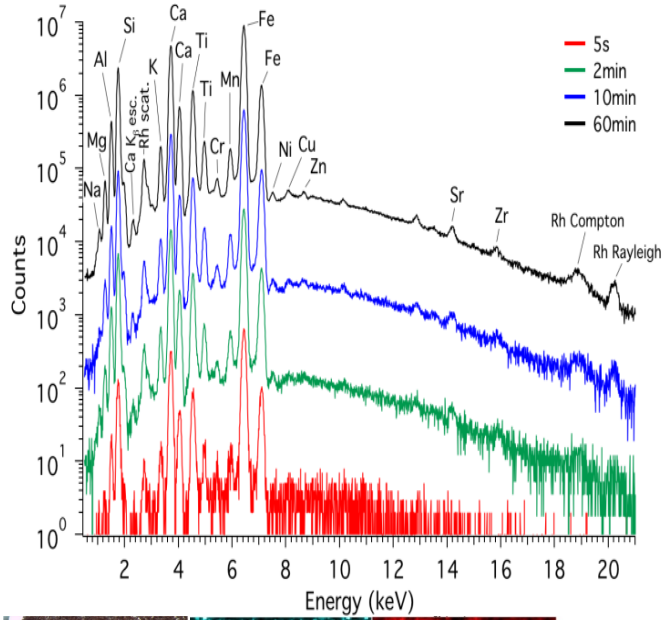
Uses a focused X-ray beam to measure the chemistry of rocks, soils

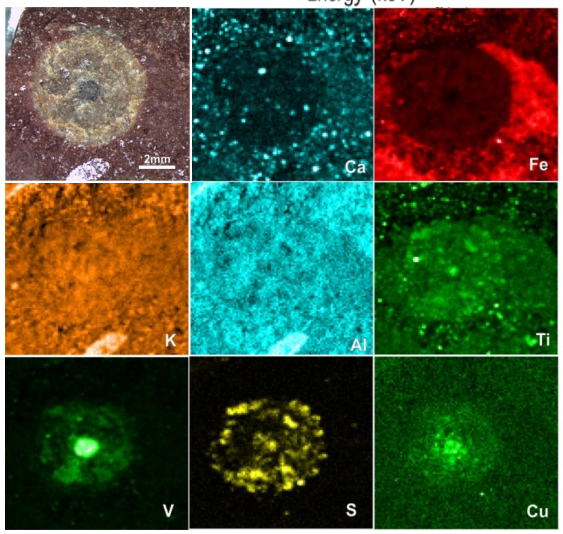
Spatial resolution (beam Ø) at focus = 0.12mm

X-Y scanning

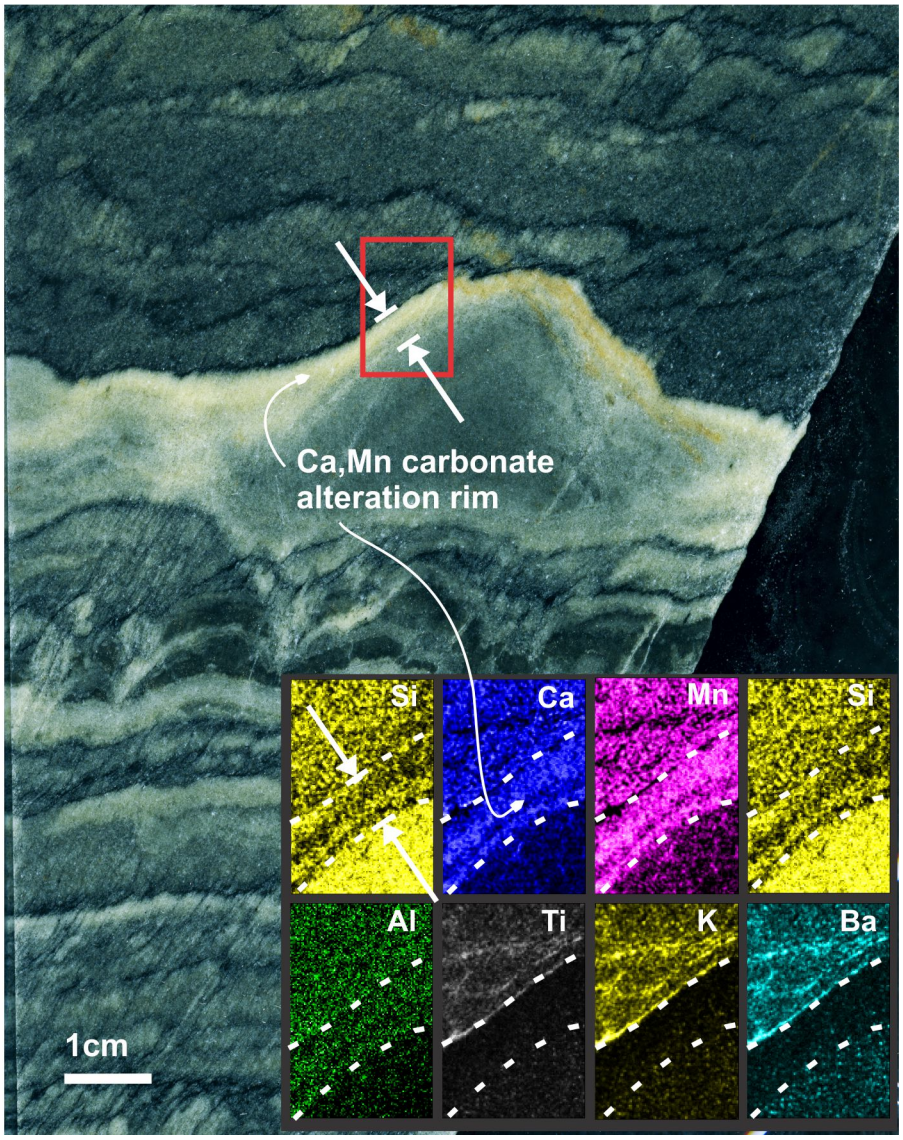
Z motion to maintain focus

optical fiducial system (OFS) for context imaging and determining X-ray beam position on target

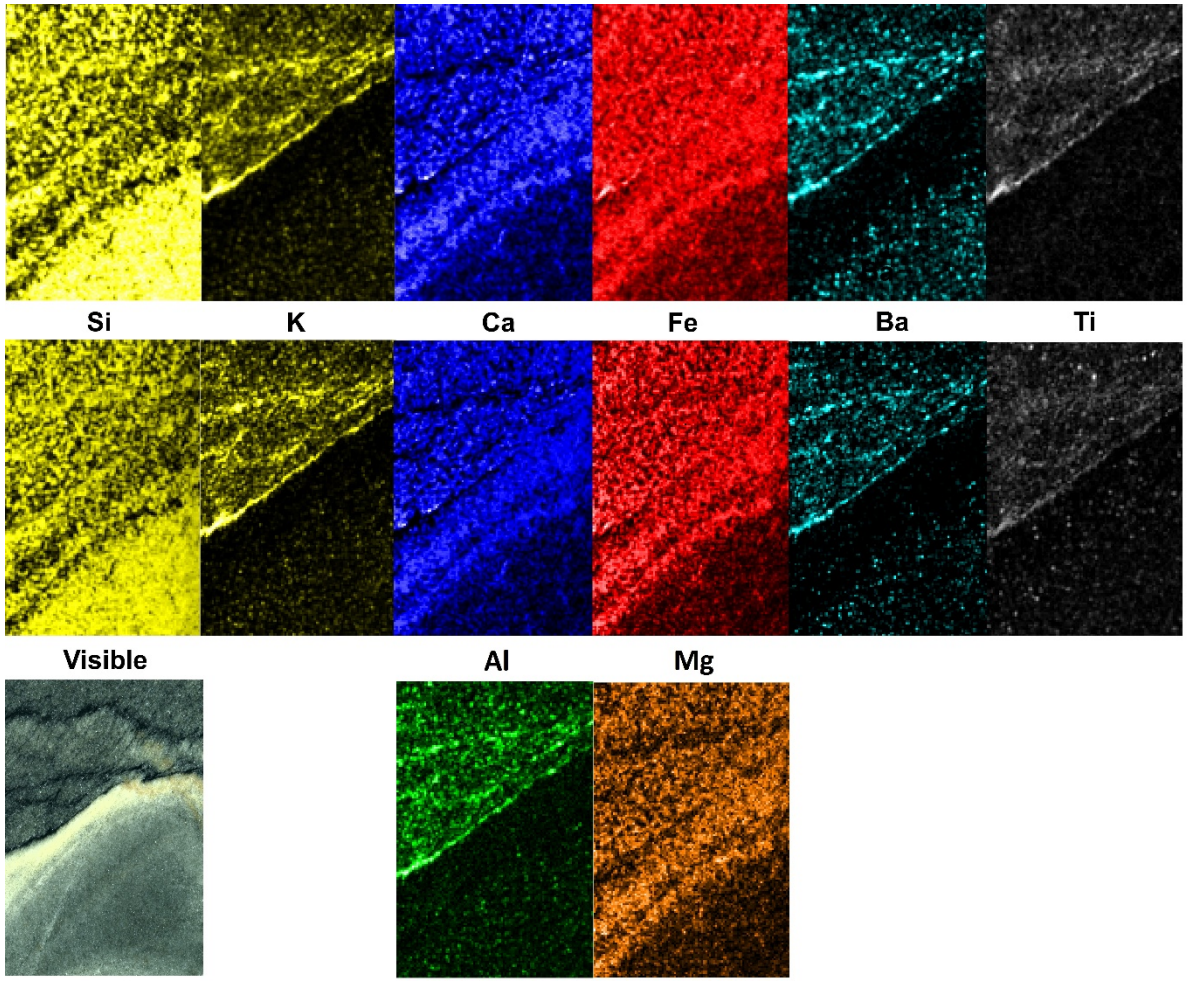




Potential biosignature and context analysis



Greenland elemental maps



Concluding remarks

- PIXL and Mars 2020 – continued discovery of Mars
  - Geological chemistry
  - Provenance – early development
  - Habitability
  - Biosignatures
  - Sample caching
  - Preparation for humans

- PIXL team efforts:
  - Ready flight instrument
  - Scientific preparedness
    - PIQUANT software
    - Elemental quantification calibration – FP approach
    - Map data visualization (eg. t-SNE)
    - Bulk quantification challenges (heterogeneities, rough surface, round edges)

Acknowledgments

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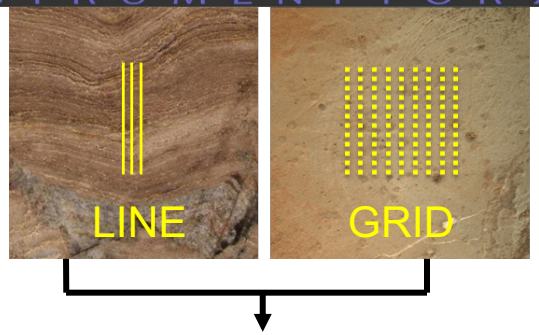
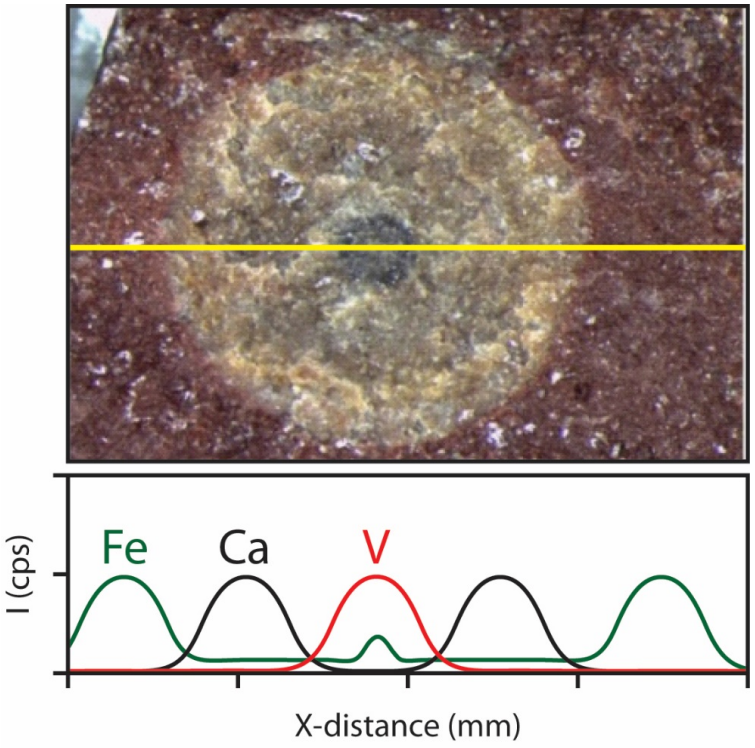
We extend our appreciation to the Denver X-ray Conference organization committee for their hard work in making this conference possible.

Thank you for listening.

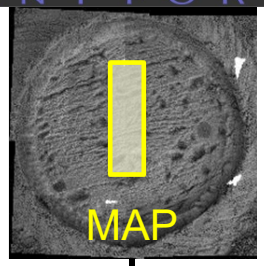
Tactical Data Products – Position vs. intensity plots





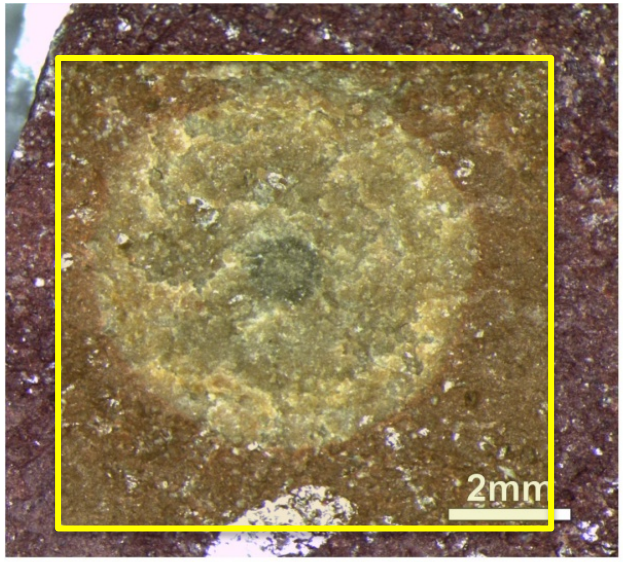
- Mosaic and register MCC images with WATSON image
- Plot PIXL scan line(s) on WATSON image
- Process spectra
- Create position versus intensity plots (correlated to Watson image) for elements with adequate SNR

Tactical Data Products – Element Intensity Maps

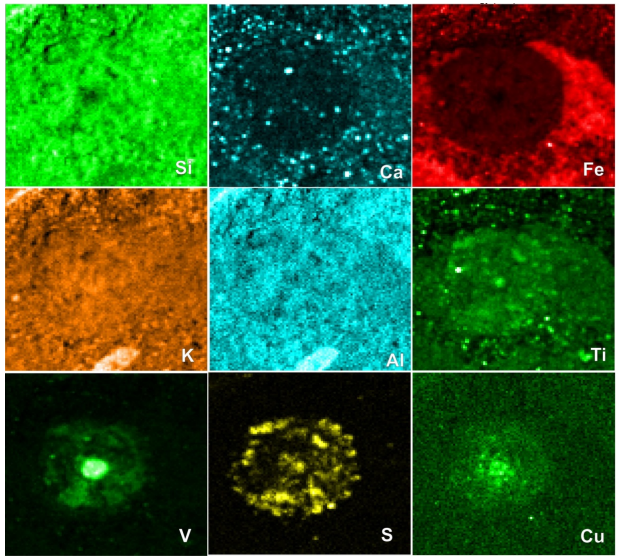


Mosaic and register MCC images with WATSON image → plot PIXL scan lines on WATSON image → Process spectra → create net intensity plots

Net Intensity Plot (correlated to WATSON image) for elements with adequate SNR



PIXL scan area on WATSON image



Net Intensity Plot